Role of MQOs in Implementation of FACDQ Candidate Detection and Quantitation Procedures

Introduction

The TWG agrees that MQOs are necessary and appropriate to calculate and characterize uncertainty at both the detection limit (DL) and quantitation limit (QL). One MQO has been considered by the TWG for detection procedures: the false positive rate. Three MQOs have been considered by the TWG for quantitation procedures: the false negative rate, accuracy and precision.

The existing system for determining detection limits (MDL) uses a false positive rate of 1%, though verification is not required. However, the existing system for determining quantitation limits (ML) does not explicitly include measurement quality objectives (MQOs) for data quality indicators, such as precision, accuracy, and false negatives (recall the ML is EPA's embodiment of a quantitation limit, QL).

The FACDQ candidate QL procedures include the use of specific values for some or all of the following MQOs, precision, accuracy and false negatives to calculate a QL, thus these MQOs define when one has reached "quantitation." Because the candidate procedures require MQOs, this document is provided by the TWG to describe for FACDQ what is meant by MQOs and how they would be used in a procedure process.

MQOs for Detection

For detection at DL, there is TWG consensus that a less than or equal to 1% false positive rate is the only appropriate MQO. A feature of the candidate detection procedures is that they also verify this consensus false positive MQO.

FACDQ Action Requested

The TWG recommends that a ≤ 1% False Positive rate be used for detection and asks the FACDQ to ratify this.

The False Negative MQO

The false negative rate (measured at L_Q relative to a detection decision at L_C) is controlled by the blank variability and/or the measurement precision at the quantitation limit and the separation between the defined detection limit (DL) and the quantitation limit (QL). If the quantitation limit is established at the detection estimate, the false negative rate for a spike at the QL will be 50% if mean recovery is 100%. Under these conditions there is a 50/50 chance that a true concentration at the QL would be "detected". If precision and bias (accuracy) remain constant the false negative rate decreases as the separation between the detection limit and the quantitation limit increases.

There are two perspectives among TWG members regarding the need to define a specific false negative rate. From one perspective, a low false negative rate is needed in order to have assurance that when the analyte of concern is present at the quantitation limit it can actually be detected. From another perspective however, accepting a higher false negative rate could mean less data censoring, since results between the DL and QL may be reported as "DNQ" (Note: FACDQ is considering a uses provision that would allow reporting of values between DL and QL in a

supplemental report). Regardless of perspective, TWG members agree that determining and/or verifying a targeted false negative rate could be impractical because of the large amount of data needed to measure that rate. Most TWG members agree that various techniques, other than specifically measuring false negative rates, could be used to control for the number of false negatives generated.

FACDQ Action Requested

If a procedure being considered for recommendation by the TWG requires the need for a targeted False Negative rate for determining the QL, what should that False Negative rate be? The TWG recommends using a False Negative rate of ≤ 5% at the detection limit for determining the quantitation limit.

MQO Continuum and MQOs for Quantitation

The following describes the continuum of how MQOs for quantitation might be set for use in the Clean Water Act program:

A. Universal, fixed MQOs for all analytical methods and analytes (for example; 5% false negatives, 20% RSD, 70-130% Recovery; assumes that false positives are already well within 1%).

B. Analyte and method specific MQOs with no upper or lower bounds.

While there is agreement within the TWG that MQOs must be established for quantitation procedures, consensus does not exist regarding their exact application, especially for accuracy and precision. The issues are:

- Without universal, fixed MQOs, QLs with different degrees of uncertainty will result.
- With universal, fixed MQOs, certain analytical methods or analyte tests would not meet those universal, fixed MQOs.

The TWG discussions led to the following findings/recommendations:

1. The MQOs for quantitation must be set someplace on the continuum between A and B.
2. Regulatory use of quantitative results will require a DQO process that specifies their appropriate application, depending upon level of uncertainty associated with the QL.

FACDQ Action Requested

1. ***The TWG asks the FACDQ to verify the above findings/recommendations and to provide specific policy input on these items.***
2. ***The TWG asks the FACDQ if they believe target precision and accuracy MQOs for the QL procedure are needed? If so, what should those MQO numbers be for Precision and Accuracy?***

The TWG strongly states that agreement on these issues is critical to recommending a final set of procedures. The TWG will make a presentation at the FACDQ to more thoroughly explain the choices.